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A new method for the determination of cooperative hydrogen bonding enthalpy of proton acceptors with associated species of alcohols

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Abstract

A calorimetric method for the determination of cooperative hydrogen bonding (HB) enthalpy of proton acceptors (B) with associated species of alcohols is proposed. The average enthalpy of cooperative HB of pyridine with associated species of alcohols was found to be -19.8 ±0.6 kJ mol-1 for all alcohols investigated. This value exceeds the enthalpy of HB in the complex ROH... N5H5 (the average for all alcohols is -15.8 ± 0.2kJ mol-1) by 20-30%. Cooperativity factors (A b, AOx) of hydrogen bonds for (ROH)2... NC 5H5 complexes were determined using the IR-spectroscopic method. The average values for the alcohols under consideration were found to be Ab = 1.41 ±0.04 and AOx = 1.54±0.05. On the basis of IR-spectroscopic and calorimetric data, the enthalpy of cooperative interactions of pyridine with the dimer (ROH)2 was estimated. This value for all the alcohols studied is, on average, -20.9 ±0.1 kJ mol -1. Copyright © 2006 John Wiley & Sons, Ltd.

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Keywords

Aliphatic alcohols, Calorimetry, Cooperativity, Enthalpy of solution, Hydrogen bonding, IR spectroscopy, Pyridine